

Supplementary data for the article:

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Supplementary Information

Thiourea based dipodal receptor development for electrochemical detection of Br⁻ ion in an aqueous medium

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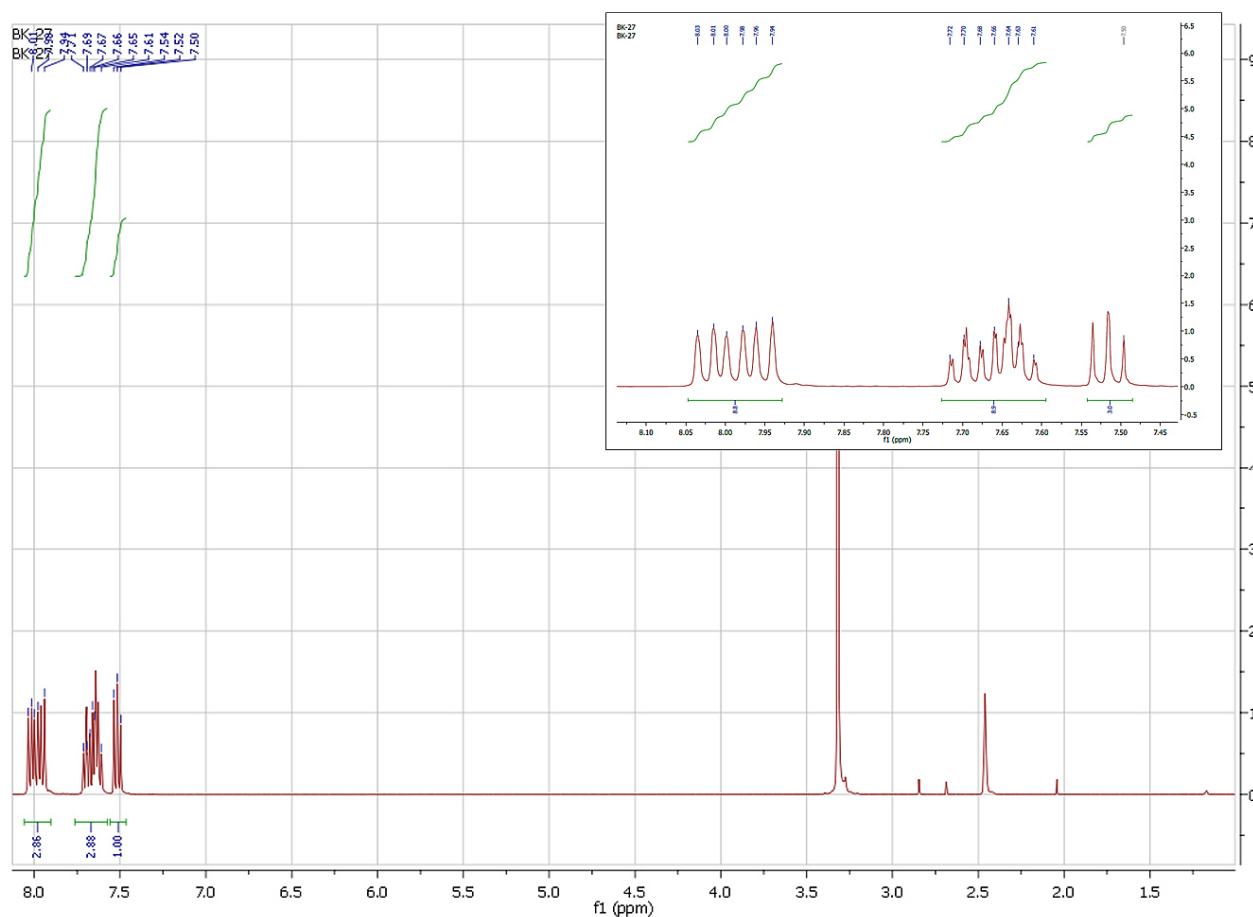
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General Information:

Sigma Aldrich Co. supplies all the chemicals of analytical grade. Solvents were purchased from SD Fine Chemicals Inc. The 400MHz and 100MHz frequency was used to obtain ^1H and ^{13}C NMR spectrum on Avance-11 (Bruker) instrument. Flash EA 1112 was undertaken for elemental analysis. Average particle size of nano particles was analysed with Metrohm Microtrac Ultra Nanotrac Dynamic Light Scattering Technique. 120KV of Hitachi instrument was utilized for taking TEM images providing resolution of 0.36nm. It confirms the size and morphology of **N1**. Waters Micromass instrument was employed for calculating mass of organic receptor synthesized. Cyclic voltammetric (CV) and Differential voltammetric studies (DPV) were performed on Epsilon BASi instrument. Studies were carried out at a scan rate of 50mV and 20mV for CV and DPV respectively. In CV and DPV 3 electrode system of Ag/AgCl wire, Pt wire and Pt disc was used to investigate determination of analyte. NaClO_4 was used as supporting electrolyte. Br^- solution was obtained in water using tetra butyl ammonium bromide salt. **R1** was fully characterized with elemental analysis.



^1H NMR (400 MHz, DMSO) δ : 7.5(t, 3H, Ar-H), 7.61-7.72(m, 9H, Ar-H), 7.94-8.03(t, 9H, Ar-H)

Figure S1. ^1H NMR spectrum for receptor **1**, inset zoomed ^1H spectra from δ : 7.5 -8.05

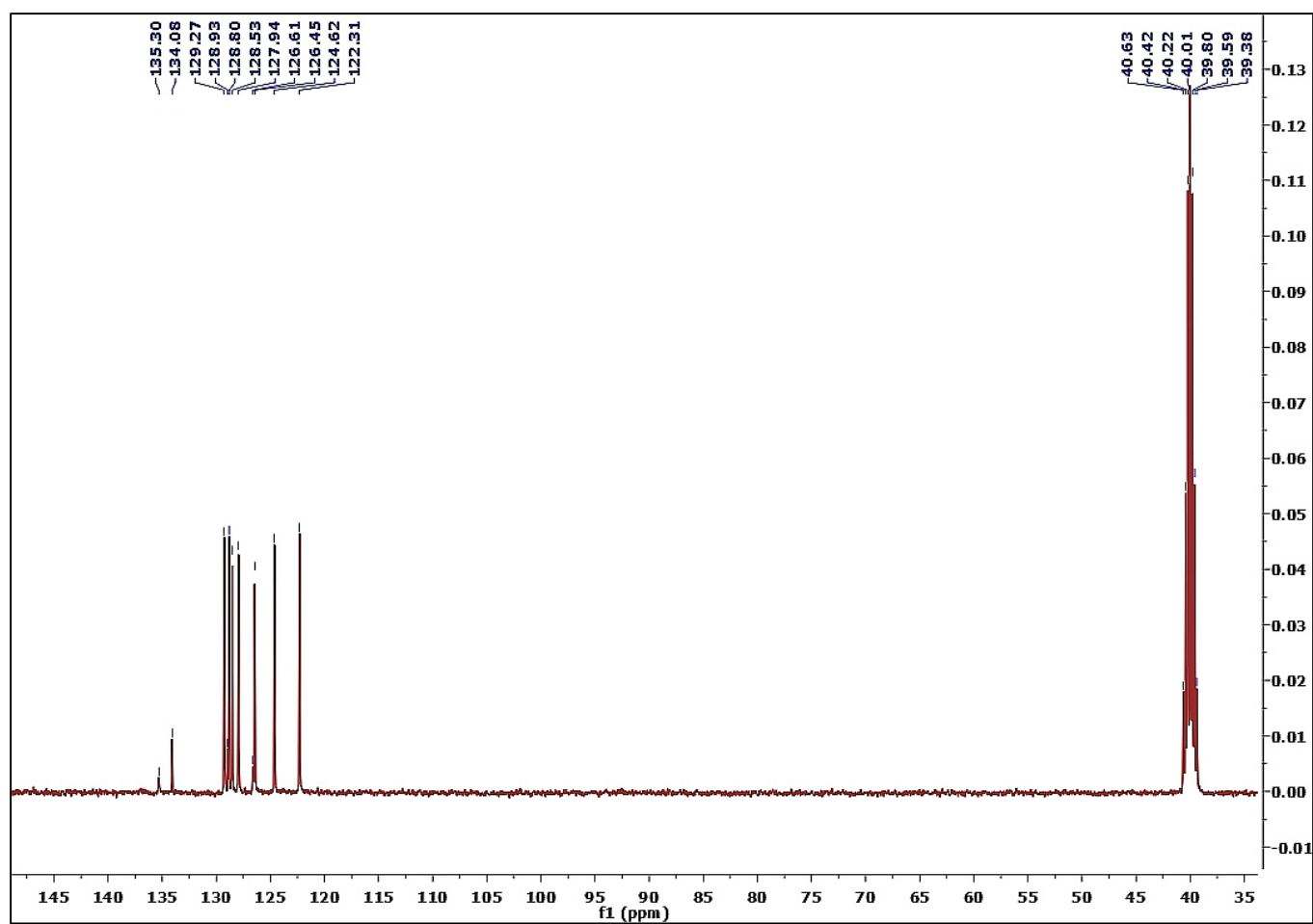


Figure S2. ^{13}C NMR spectrum for receptor **1**

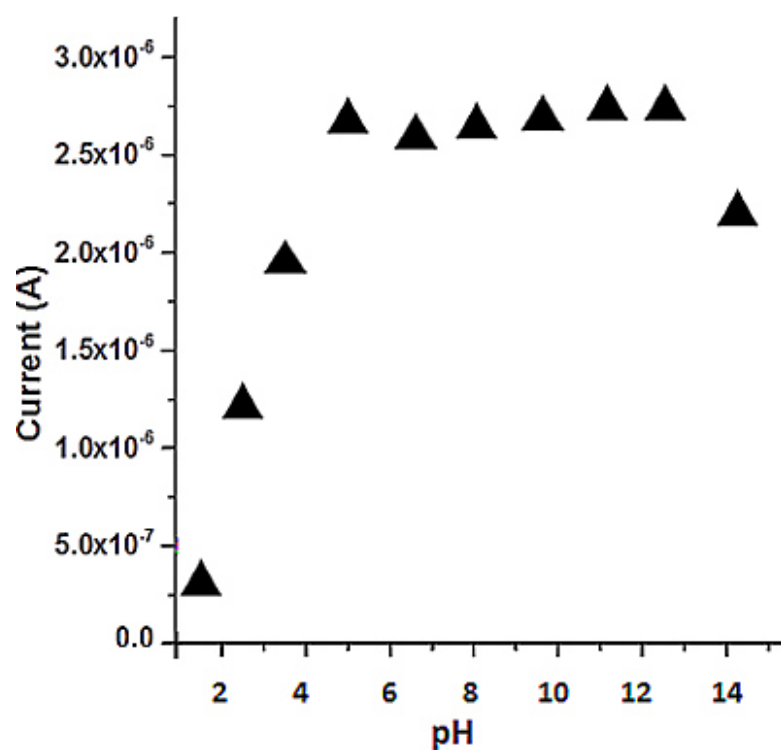


Figure S3. Plot of current intensity obtained for **N1.Br⁻** at different pH values

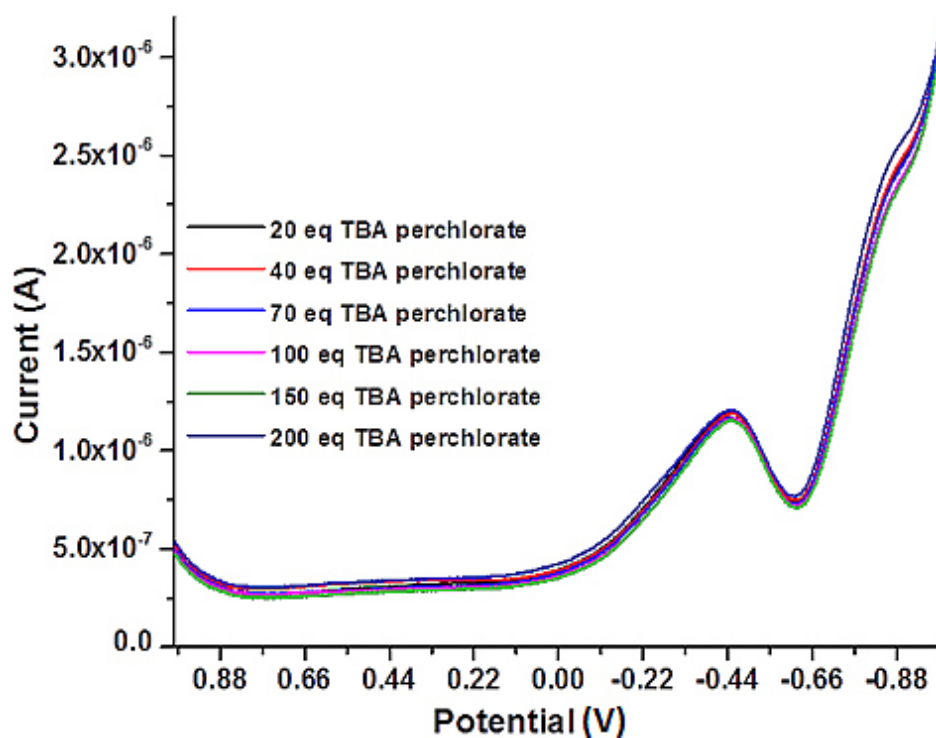


Figure S4. Effect of ionic concentration on DPV profile of **N1.Br⁻** with addition of tetrabutylammonium salt of perchlorate (0-200 equiv.) in the solution of **N1.Br⁻**

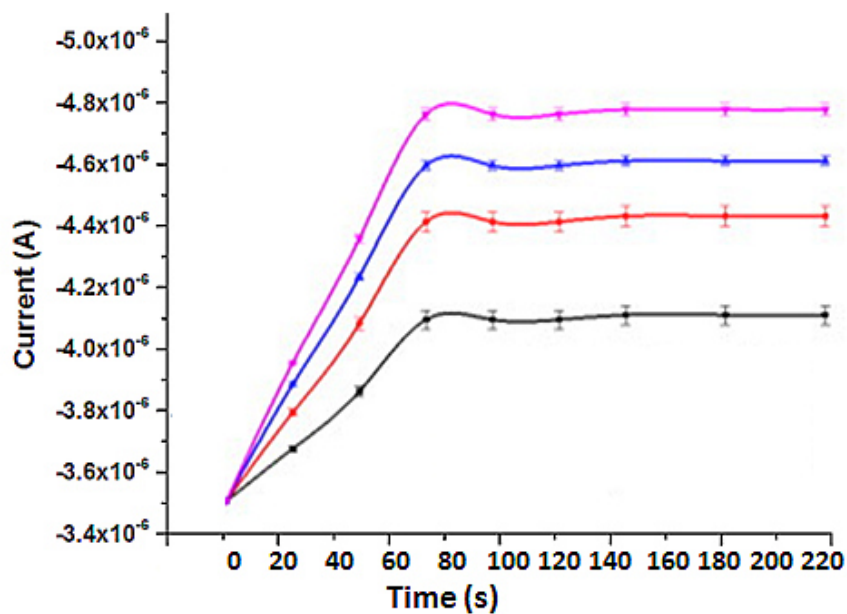


Figure S5. Plot of DPV profile of **N1.Br⁻** with various concentrations as a function of time in seconds in the solution of **N1.Br⁻**

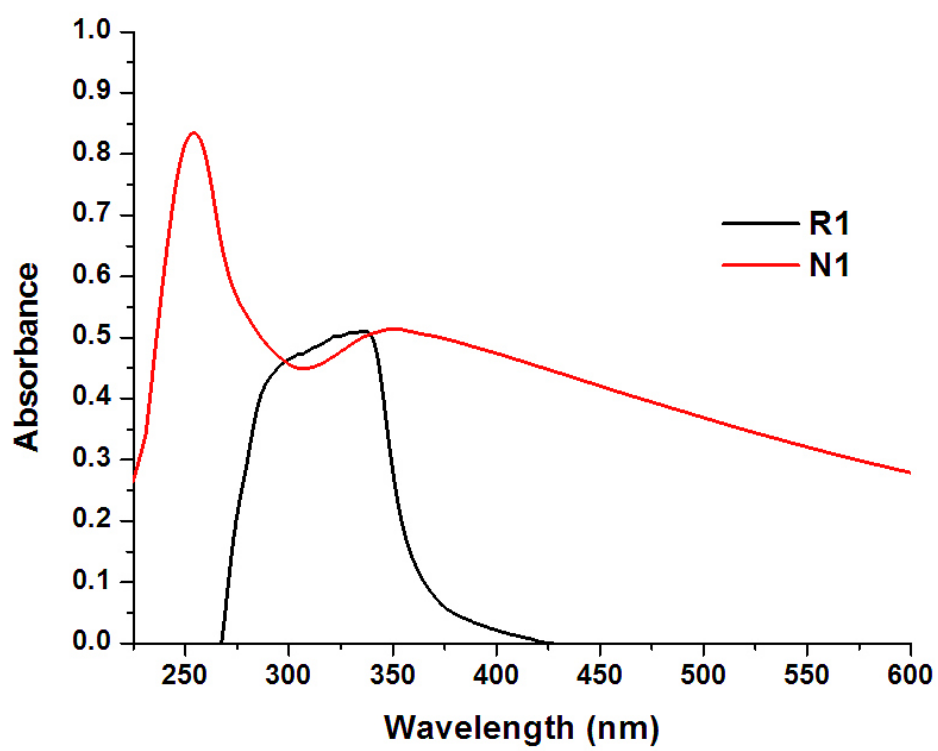


Figure S6. UV-Vis absorption spectra of **R1** and **N1**

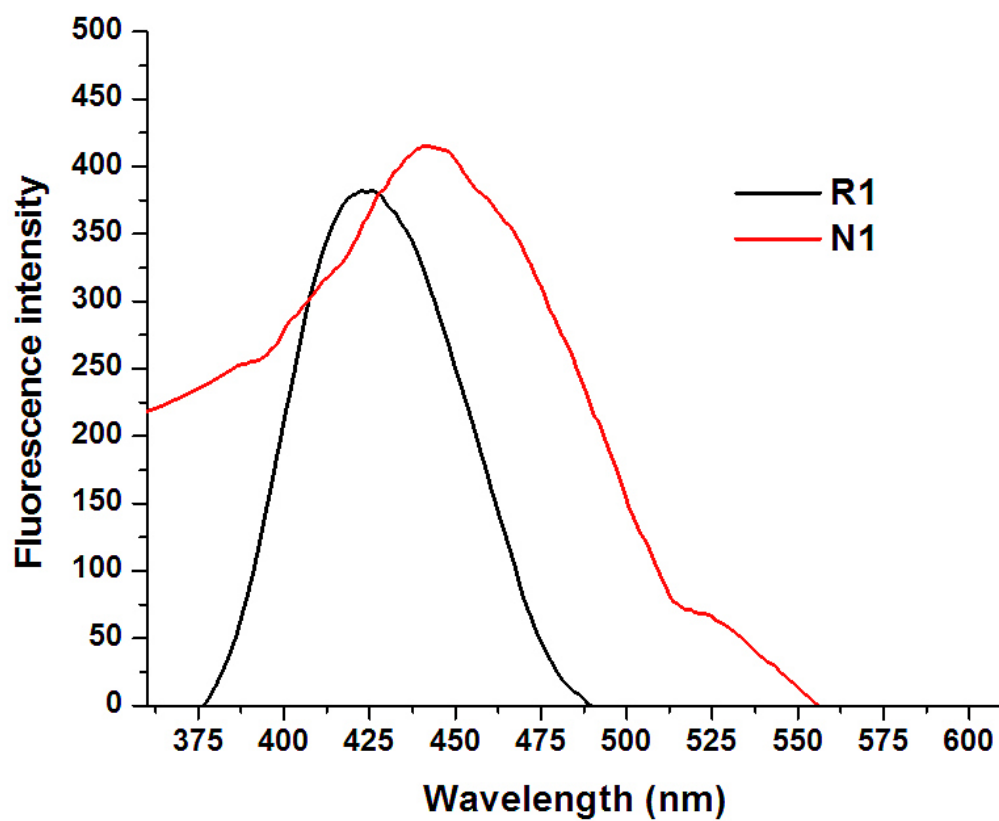


Figure S7. Fluorescence emission profile of **R1** and **N1**

Table S1: Comparison of proposed sensor with some of reported sensors for bromide using various analytical techniques

S. No.	Journal	Method	Medium	Detection range	Detection limit	Inter ference	Application explored	Referen ce
1	Sensors and Actuators B	Ion Selective electrode	Aqueous	$10^{-1} - 10^{-2}$ M	1.6×10^{-5} M	Not mentioned	Not mentioned	30
2	Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy	Electrochemical	Aqueous	7.0×10^{-6} - 1.0×10^{-1} M	6.0×10^{-6} M	No interference	Not done	31
3	Journal of Electroanalytical Chemistry	Electrochemical	Aqueous	$0.01 - 1 \mu\text{M}$	1.0×10^{-8} M	Not done	Water samples	32
4	Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy	Calorimetric, UV	Aqueous		$1.67 \mu\text{M}$	No interference	Not Done	33
5	Biosensors and Bioelectronics	Electrochemical	Aqueous	$10^{-7} - 10^{-1}$ M	63nM	Biosensors and Bioelectronics	Human plasma, urine	34
6	Electro analysis	Electrochemical	Aqueous	0-100 μM	3.79nM	No interference	Water samples	Proposed sensor